

The paramagnetic and glass transitions in sudoku

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We study the statistical mechanics of a model glassy system based on a familiar and popular mathematical puzzle. Sudoku puzzles provide a very rare example of a class of frustrated systems with a unique groundstate without symmetry. Here, the puzzle is recast as thermodynamic system where the number of violated rules defines the energy. We use Monte Carlo simulation to show that the “Sudoku Hamiltonian” exhibits two transitions as a function of temperature, a paramagnetic and a glass transition. Of these, the intermediate condensed phase is the only one which visits the ground state (i.e. it solves the puzzle, though this is not the purpose of the study). Both transitions are associated with an entropy change, paramagnetism measured from the dynamics of the Monte Carlo run, showing a peak in specific heat, while the residual glass entropy is determined by finding multiple instances of the glass by repeated annealing. There are relatively few such simple models for frustrated or glassy systems which exhibit both ordering and glass transitions, sudoku puzzles are unique for the ease with which they can be obtained with the proof of the existence of a unique ground state via the satisfiability of all constraints. Simulations suggest that in the glass phase there is an increase in information entropy with lowering temperature. In fact, we have shown that sudoku have the type of rugged energy landscape with multiple minima which typifies glasses in many physical systems, and this puzzling result is a manifestation of the paradox of the residual glass entropy. These readily-available puzzles can now be used as solvable model Hamiltonian systems for studying the glass transition.

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Complex systems such as glasses are typified by frustrated interactions which cannot be simultaneously satisfied. By contrast, systems with a well defined ground state are typified by some translational symmetry and long ranged ordering. The popular mathematical puzzle sudoku lies intermediate between these two. Standard sudokus, printed by the thousand in newspapers around the world, have a unique solution which normally has no symmetry. Adding one “wrong” number-constraint tips the problem into the regime of the frustrated system, which cannot be solved, while removing one of the clues leads to a system with multiple solutions.

We obtained our sudoku puzzles from the online Playr site[1], and also investigate a minimal 17-clue puzzle[2] Overconstrained and underconstrained puzzles were created by adding or removing constraints from these puzzles. For human solution, the puzzle should be solved by “logic”, and puzzles are categorized by how difficult it is to do this. The Playr site rates puzzles on a five-point scale.

The sudoku problem can be cast into a Hamiltonian form. Here a 9x9 grid contains “spins”, taking integer values between 1 and 9. The sudoku rules require that no “spins” in the same row, column or 3x3 sub-grid should take the same value. By assigning an energy to each violation of the rules, we arrive at the following Hamiltonian

$$H = \sum_i H(\{\sigma_i\}) = \sum_i \sum_j \delta_{\sigma_i \sigma_j} \quad (1)$$

Where the j sum runs over all sites which share a row, column, or sub-grid with i . The problem is defined by

assigning fixed values to some spins (“clues”), and treating the others as dynamic variables. The solution to the sudoku problem is the ground state of the Hamiltonian, which has $H = 0$. It can be seen that this is equivalent to a 9-state Potts Hamiltonian on a 20-neighbour finite periodic lattice.[3]

Here, we define microstates of the system with each σ_i taking a value between 1 and 9. We then sample the microstates according to the Boltzmann distribution with a fictitious temperature, T [4], i.e. the probability of a state with energy H is $p(H) \sim \exp(-H/T)$. This is done by accepting or rejecting trial changes of individual numbers using the Metropolis algorithm[5]. This Markov process could be set to terminate once $H = 0$, acting as a solver, however better methods are available for solving sudoku puzzles[6–8] and this is not the purpose of this work. We are interested in the equilibrium macrostate and glassy dynamics so we will use the Monte Carlo simulation to obtain ensemble averages.

The mean energy $\langle H \rangle$ was evaluated, and the specific heat

$$c_v = \langle (H - \langle H \rangle)^2 \rangle / T^2 \quad (2)$$

for representative problems are shown in figure 1. This shows a transition between a low temperature “ordered” state close to the ground state, and a high temperature “paramagnetic” state with many rule violations. The variance of the energy shows a distinct peak at this temperature. These are the classic signals of a phase transition, and hereinafter we will refer to it as such, however we note that since the system size is fixed there is no “thermodynamic limit”. For a system of this small finite

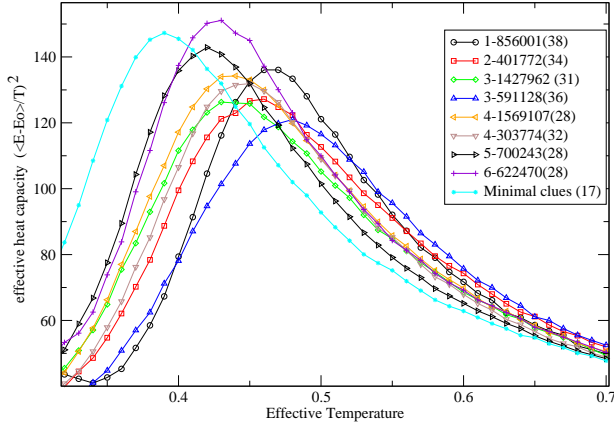


FIG. 1: Variation of “heat capacity” with temperature, showing that the transition temperature shifts with number of fixed values. Legend shows the Playr puzzle number, with the first digit labelling the “difficulty” and the number in brackets the number of fixed sites.

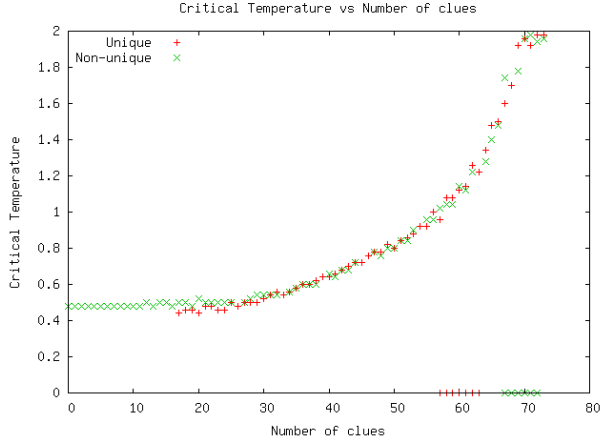


FIG. 2: Variation of critical temperature with number of clues for puzzles with and without unique solutions.

size, we expect such a rounded peak rather than a discontinuity. Larger sudoku puzzles with 4x4 and 5x5 grids exist, but the Potts-model sites have more neighbours, so do these not comprise a limit. The finite size of the phase space means that peaks are rounded rather than sharp, and consequently we were also unable to obtain sufficient data to calculate critical exponents.

The transition temperature shows a strong dependence on the number of fixed sites, but not on the existence of a unique ground state solution (Figure 2). We investigated this by taking published puzzles, and either fixing additional sites (consistent with the solution) to increase that number, or removing fixed sites to create systems with multiple minima, or both.

Two phases discovered here are akin to a high entropy paramagnetic phase, which samples the whole phase space, and an ordered condensed phase which is close to

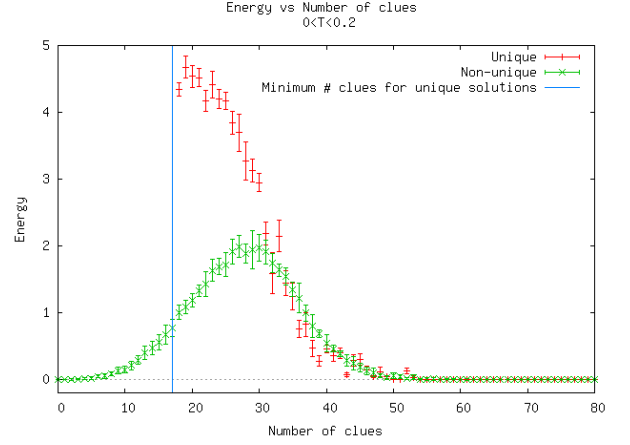


FIG. 3: Variation of mean energy in the $T < 0.2$ range for a series of puzzles with different number of fixed sites, showing the appearance of a glassy state for intermediate numbers of clues, and an increased tendency towards glassiness for puzzles with a unique solution

the solution, while sampling other well-defined, energy minimum. The ground state, while unique, has no symmetry, and there are also other macrostates corresponding to metastable energy minima in which the system can become stuck at low temperature. We refer to the phase stuck in this rough non-symmetric energy landscape as a glass.

We studied a number of systems and monitored their ensemble average low T energy after an equilibration time of 200000 MC steps (Fig 3). In general, this places us in a non-ergodic regime with each simulation becoming fixed in a local minimum. It is therefore a kinetic rather than thermodynamic measure, the non-zero values of $\langle H \rangle$ being due to failing to find the global minimum below the glass transition rather than thermal noise. For puzzles with multiple solutions the maximum complexity (as measured by mean low temperature energy) appears with about 27 fixed sites. With more fixed sites there is a smaller phase space, and the ground state is quickly found. With fewer clues, there is an increasing number of zero energy states, and again one is easily located. This may be regarded as a degenerate glass.

This latter argument does not hold for puzzles with a unique solution, where equilibration from an initial random state typically falls into a local minimum. Indeed we see that the low-temperature ensemble-averaged energy for systems with unique solution increases sharply towards 17, the minimum possible[9].

The existence of a unique ground state makes it possible to be certain when the simulation is in a metastable state close to a non-zero-energy minimum. From this it is also possible to probe the roughness of the energy landscape and determine something analogous to a glass transition. At very low temperature the simulation falls

into a local minimum and becomes stuck. Then on heating we enter the “glassy” regime where a variety of different states are sampled, including the ground state. This transition is associated with a broad peak in the specific heat on the c_v vs T plot, but a clearer measure of the number of local minima can be determined by measuring the fraction of time that the system is in the ground state (Fig.4). We find that there is a correlation between both “difficulty” rating and number of fixed sites for the number of metastable states: harder puzzles with fewer clues spend less time in the global minimum, and therefore more in metastable minima. By contrast, the peak always falls at the same temperature, showing that the energy barriers between the various local minima are similar in all puzzles.

The existence of a particular temperature which is optimal for finding the ground state implies that both above and below this temperature, the entropy of the system should be higher. This is a more extreme case of the residual entropy of glass and disordered crystals[10, 11] in that the sudoku system appears to show a negative dS/dT . Such a result, if converted from statistical mechanical entropy to thermodynamic entropy, would imply a violation of the second law. However there is no physical representation of this system, and no reversible process equating to our simulation, so the issue is mainly one of definition of entropy.

The information (Shannon) measure is the “configurational entropy” of the system, defined as:

$$S = - \sum_{i,j,k}^9 p(\sigma_{i,j} = k) \ln p(\sigma_{i,j} = k) \quad (3)$$

where $p(\sigma_{i,j} = k)$ is the ensemble-averaged probability of finding the number k at site (i,j) . In calculating this entropy, the process for evaluating the “ensemble average” becomes critical. $S(T)$ is relatively featureless when calculated from a single long trajectory at each temperature, decaying monotonically to $S=0$ at $T=0$. When averages for p_i are taken over a set of separate simulations (i.e. repeatedly annealing to high- T) a distinct entropy minimum is revealed at the glass transition, caused by the excess entropy from counting multiple instances of the glass at lower temperatures. The variation of $S(T)$ with temperature calculated in this way is shown in Fig4 (inset). It can be seen that this minimum corresponds to the peak in finding solutions, and is strongly correlated with the “difficulty” rating of the puzzle: harder puzzles have more local minima.

For an abstract puzzle like sudoku there is no “physically correct” way of evaluating the ensemble average. All we can say is that the ergodic hypothesis is clearly violated, and with it the link between statistical mechanics and thermodynamics.

To summarise, we have shown that the sudoku puzzle can be used to define a model Hamiltonian system with

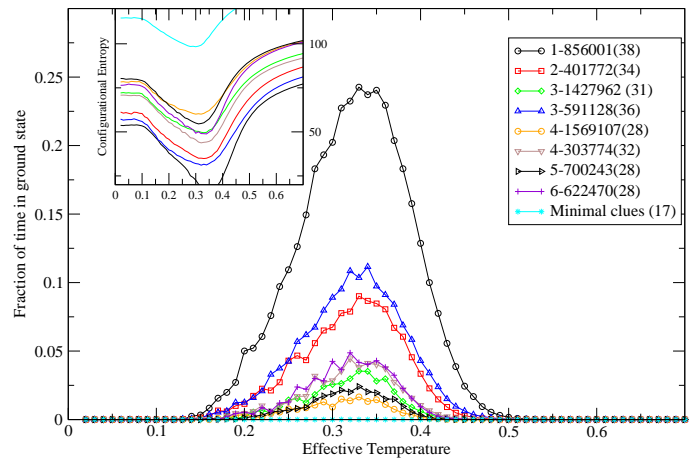


FIG. 4: Fraction of time spent in ground state for a series of puzzles with different “difficulty” rating, at each temperature, we simulated 10^9 attempted steps, split into 1000 groups with each group initially randomized, and statistics gathered over the final 8×10^5 steps. Legend shows playr puzzle number[1]. The solution to the 17 clue minimal puzzle was only found once. Inset: $S(T)$ vs T . This quantity is normalized to the number of sites, rather than the number of free sites, hence systems with a large number of free sites tend to have higher $S(T)$ throughout.

interesting properties. It exhibits three phases, paramagnetic, condensed and glass. The paramagnetic transition has a critical temperature which depends only on the fraction of fixed sites in the system. At low temperatures there is a notable difference between true sudoku puzzles with unique solutions, and the equivalent constrained Potts models with multiple solutions: the sudoku puzzles are much stronger glass-formers. Finally, the sudoku Hamiltonian sheds light on the residual glass-entropy, by providing a model in which ergodicity breaking is manifest, leading to different results for the low-temperature entropy depending on the method of simulation.

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- [1] Playr Sudoku [Online] (Accessed Mar 2012) <http://www.playr.co.uk/sudoku/index.php>. Puzzles used: 1-271179, 2-515887, 3-571356, 4-117730, 5-640430.
 - [2] The pattern of clues in this puzzle is
.....1.....2...3...4.....5...4.16.....71.....5....2.....8..4..3.91....
 - [3] Potts, R. B. (1952). Mathematical Proceedings 48 (1): 106109
 - [4] For convenience, we define units such that $k_B = 1$.
 - [5] Metropolis, N.; Rosenbluth, A. W.; Rosenbluth, M. N.; Teller, A. H. and Teller, E. (1953). J. Chem. Phys. 21, 1087-1092
 - [6] Gunther, J.; Moon, T.; (2012), "Entropy Minimization for Solving Sudoku," Signal Processing, IEEE Transactions 60, no.1, 508-513
 - [7] Babu, K. Pelckmans, P. Stoica, and J. Li, (2010) Linear systems, sparse solutions, and Sudoku, IEEE Signal

- Process. Lett., 17, 4042
- [8] Knuth, D (2000). Millenial Perspectives in Computer Science. P159 187 (2000).
- [9] McGuire, G; Tugemann, B and Civario, G. (2012) arXiv:1201.0749
- [10] E. D. Eastman and R. D. Miller, J. Chem. Phys. 1, 444 (1933); F. Simon, Physica (Amsterdam) 9, 1089 (1937).
- [11] M.Goldstein, J. Chem. Phys. 128, 154510 (2008)